alpha-d-glucopyranose 492-62-6 | DTXSID30197710

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 8.21

Global applicability domain: Outside

Local applicability domain index: 7.87e-02

Confidence level: 3.67e-01

Nearest Neighbors from the Training Set

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4-Hydroxybenzoic acid

Measured: 8.08 Predicted: 7.78

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Salicylic acid

Measured: 7.44 Predicted: 7.60

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Phenacetin

Measured: 9.59 **Predicted:** 9.23

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Methylparaben Measured: 8.57 Predicted: 7.06 Image not found

Diphenylamine Measured: 7.64 Predicted: 8.73